Research Interests in the Properties of Energetic Materials

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Our Goal

- To develop state-of-the-art methods for first-principles calculations of the physical, mechanical, and dynamical properties of polyatomic molecular systems, with special emphasis on condensed-phase energetic materials

Areas of Principal Interest (I)

- Molecular potential-energy functions
- Decomposition rates and mechanisms
- Physical and mechanical properties
- Transport coefficients

Areas of Principal Interest (II)

- Molecular energization mechanisms
- Fracture / failure of energetic material crystals
- Grain-grain and grain-binder interactions
- Aging effects in energetic materials

Molecular Potential-Energy Functions

- Fundamental to most molecular dynamics and Monte Carlo studies
- Potentials largely determine the results
- Several in existence, but of uncertain applicability to high-explosive systems
- Most often calibrated for “low” temperatures and pressures

Decomposition Rates and Mechanisms (I)

- Needed for microscopic kinetic modeling
- Both gas- and condensed-phase processes of interest
  - gas-phase methods provide useful starting point
  - major interest lies in methodological development for condensed phases

Decomposition Rates and Mechanisms (II)

- Several approaches viable
  - various flavors of transition-state theory
  - classical trajectories
  - molecular dynamics
  - quantum molecular dynamics
  - mixed classical/quantum molecular dynamics

Physical and Mechanical Properties (I)

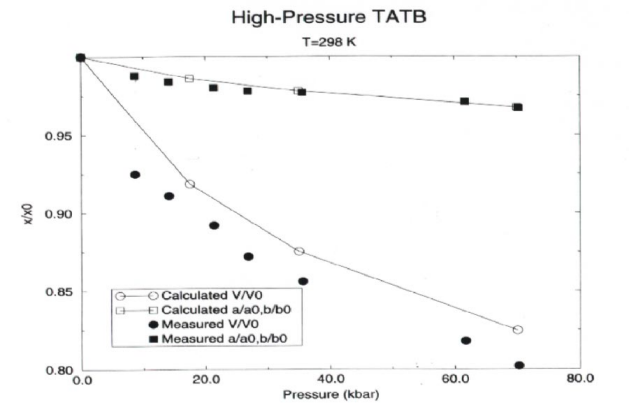
- Needed for higher-level modeling efforts
  - often used directly in micromechanical studies
  - indirect application in development of constitutive relations for continuum simulations
- Both solids and liquids are of interest

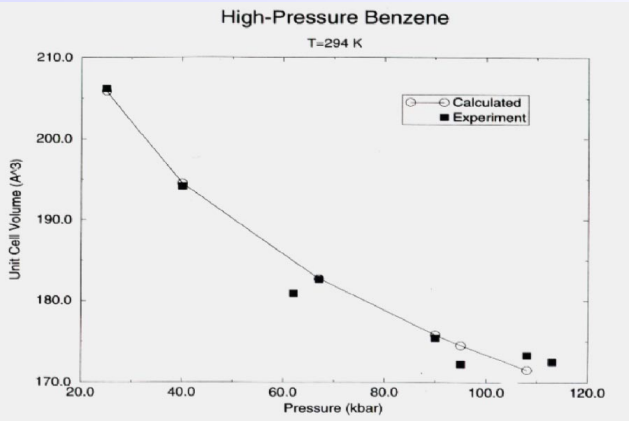
Physical and Mechanical Properties (II)

- Data needed over a wide domain of temperatures, pressures, and strain rates
  - $185\ K \leq T \leq O(10^3)\ K$
  - $0\ kbar \leq P \leq 300\ kbar$
  - $10^{-3} \leq d\varepsilon / dt \leq 10^6$

Physical and Mechanical Properties (III)

- Density as f(T,P)
- Lattice parameters
- Energy as f(T,P)
- Specific Heat
- ΔH_{fusion}
- T_{melt}

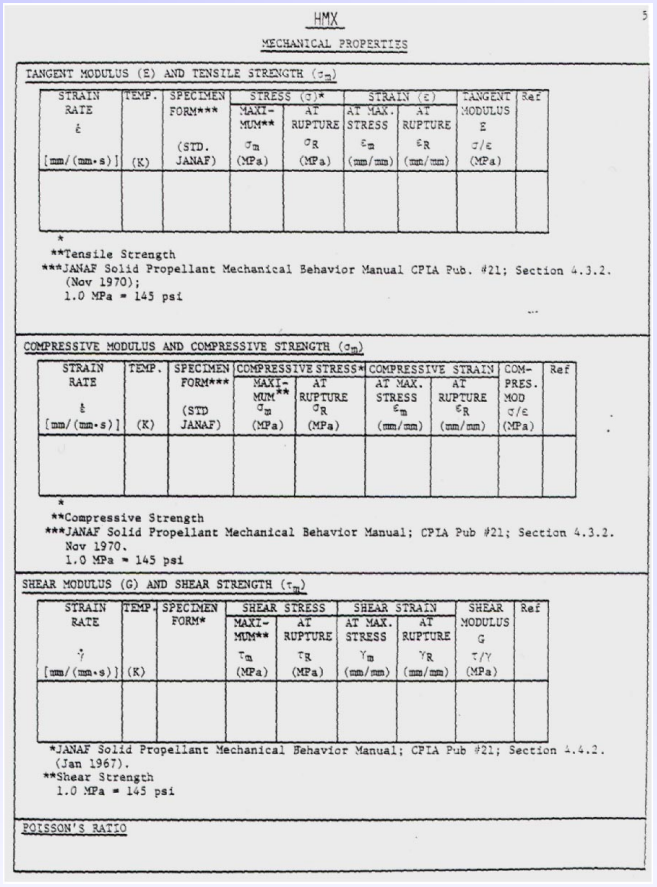




Physical and Mechanical Properties (IV)

- elastic constant matrix as f(T,P)
- derived moduli
- stress-strain behavior
- ultimate strength
- friction coefficients

HMX Data Sheet (Navy)



HMX

MECHANICAL PROPERTIES

TANGENT MODULUS (E) AND TENSILE STRENGTH (σ_m)

STRAIN RATE $\dot{\varepsilon}$ [mm/(mm·s)]	TEMP. (K)	SPECIMEN FORM*** (STD. JANAF)	STRESS (σ)* MAXIMUM** σ_m (MPa)	STRESS (σ)* AT RUPTURE σ_R (MPa)	STRAIN (ε) AT MAX. STRESS ε_m (mm/mm)	STRAIN (ε) AT RUPTURE ε_R (mm/mm)	TANGENT MODULUS E σ/ε (MPa)	Ref

*
**Tensile Strength
***JANAF Solid Propellant Mechanical Behavior Manual CPIA Pub. #21; Section 4.3.2. (Nov 1970);
1.0 MPa = 145 psi

COMPRESSIVE MODULUS AND COMPRESSIVE STRENGTH (σ_m)

STRAIN RATE $\dot{\varepsilon}$ [mm/(mm·s)]	TEMP. (K)	SPECIMEN FORM*** (STD JANAF)	COMPRESSIVE STRESS* MAXIMUM** σ_m (MPa)	COMPRESSIVE STRESS* AT RUPTURE σ_R (MPa)	COMPRESSIVE STRAIN AT MAX. STRESS ε_m (mm/mm)	COMPRESSIVE STRAIN AT RUPTURE ε_R (mm/mm)	COMPRES. MOD σ/ε (MPa)	Ref

*
**Compressive Strength
***JANAF Solid Propellant Mechanical Behavior Manual; CPIA Pub #21; Section 4.3.2. Nov 1970.
1.0 MPa = 145 psi

SHEAR MODULUS (G) AND SHEAR STRENGTH (τ_m)

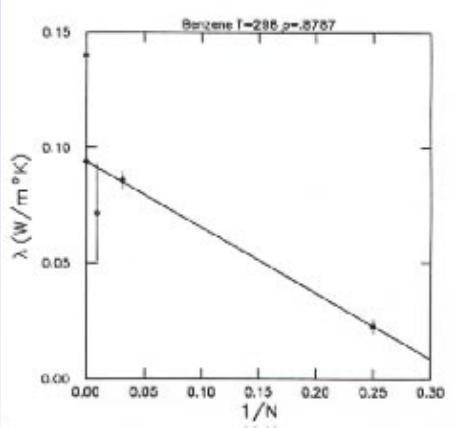
STRAIN RATE $\dot{\gamma}$ [mm/(mm·s)]	TEMP (K)	SPECIMEN FORM*	SHEAR STRESS MAXIMUM** τ_m (MPa)	SHEAR STRESS AT RUPTURE τ_R (MPa)	SHEAR STRAIN AT MAX. STRESS γ_m (mm/mm)	SHEAR STRAIN AT RUPTURE γ_R (mm/mm)	SHEAR MODULUS G τ/γ (MPa)	Ref

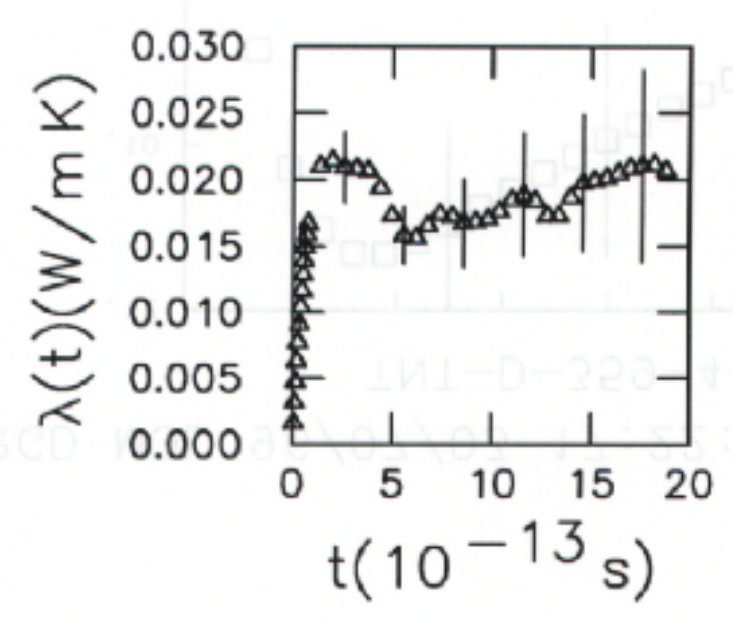
*JANAF Solid Propellant Mechanical Behavior Manual; CPIA Pub #21; Section 4.4.2. (Jan 1967).
**Shear Strength
1.0 MPa = 145 psi

POISSON'S RATIO

Transport Coefficients

- shear viscosity as f(T,P)
- thermal conductivity
- diffusion





Molecular Energization Mechanisms (I)

- Relevant to microscopic theories of initiation
- Dynamics in shocked / strained crystal
- Intra- and intermolecular energy transfer pathways and rates

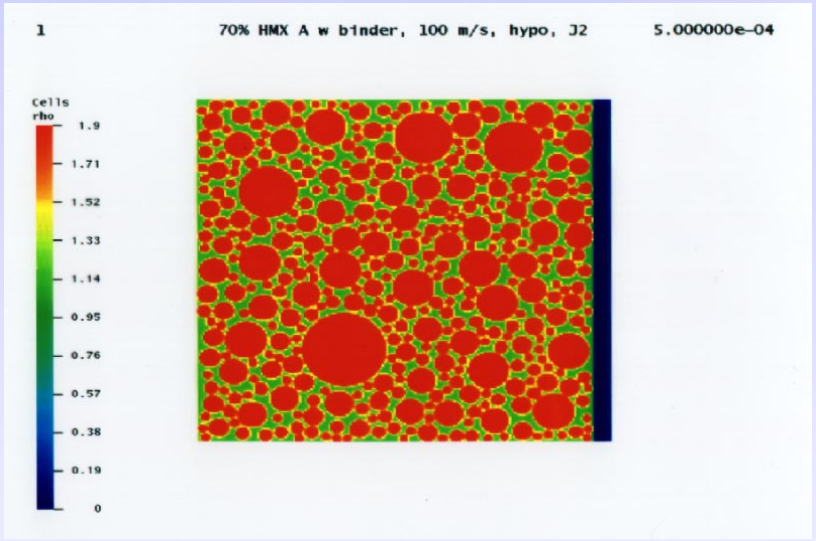
Fracture/Failure of Energetic Material Crystals

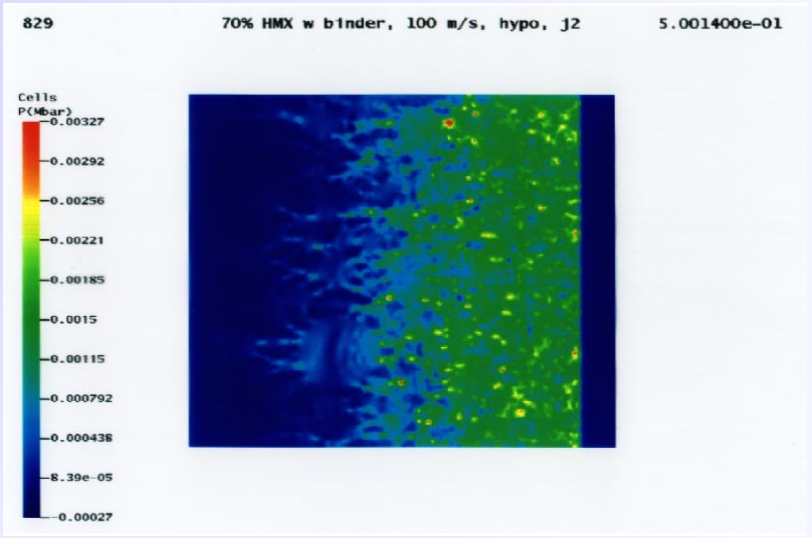
- Direct simulation of microscopic crack propagation
- Energy dissemination at crack tip
- Failure mechanism (strain-rate dependence?)

Grain-Grain and Grain-Binder Interactions

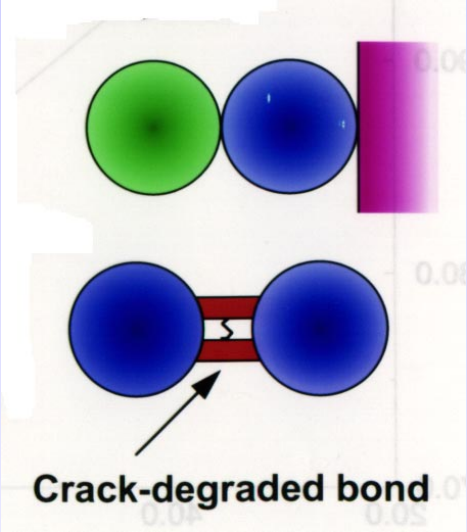
- Predominantly non-atomistic approaches
  - Discrete Element Method (DEM)
  - Fluid-Implicit Particle (FLIP) method
- Heavily reliant on input from atomistic-level results

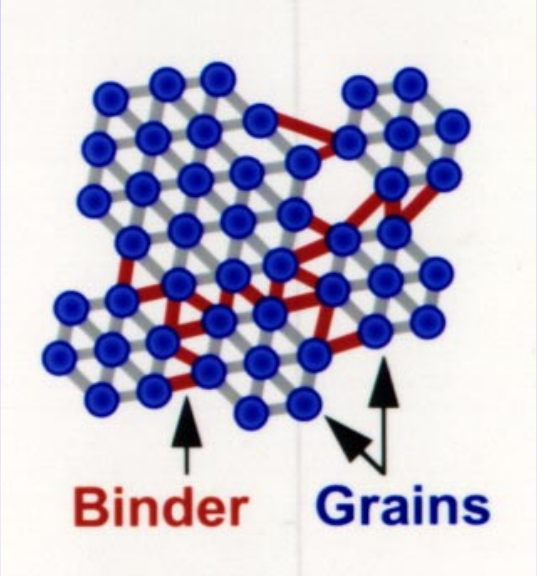
Sample FLIP Calculation

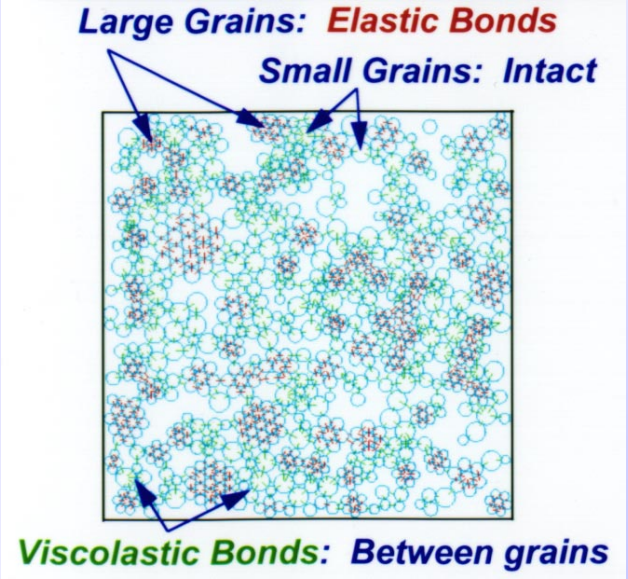




Discrete Element Model







Aging Effects in Energetic Materials (I)

- Safety, reliability, and performance
- Areas of potential concern
  - chemical degradation of explosive molecules
  - changes in binder materials
  - dewetting of HE crystallites

Aging Effects in Energetic Materials (II)

- Effects of HE decomposition on surrounding materials
- Effects of binder aging on mechanical properties and viscoelastic response
- Effects of dewetting on structural integrity of the composite

Summary

- Need an improved, science-based understanding of energetic material systems
- Computational science is an important component of the solution
- ASCI/ASAP provides an attractive mechanism for approaching the problem